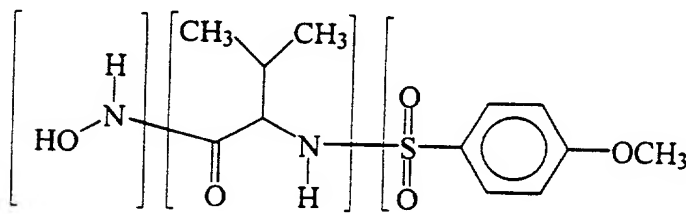
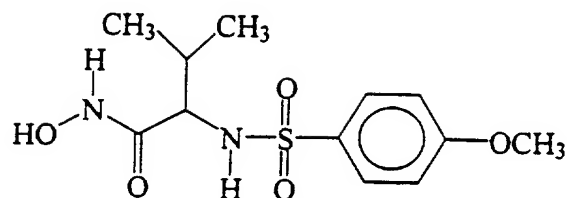


Compound CI



	Fi	Fii	Fiii
Molecular formula	H_2NO	C_5H_9NO	$C_7H_7O_3S$

Figure 1

Addition of fragments to yield compounds

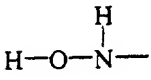
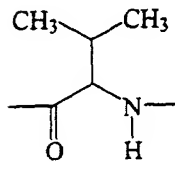
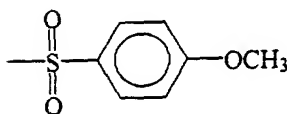
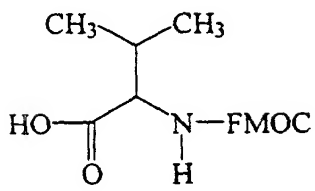
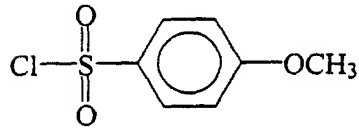
Fragment Identifier	Table			
	Structure	Name	Molecular formula	Other
F _i		Hydroxylamine	H ₂ NO	...
F _{ii}		Amino acid	C ₅ H ₉ NO	...
F _{iii}		Sulfonyl	C ₇ H ₇ O ₃ S	...

Figure 2

Reagents	Identifier	Name	Properties
$\text{H}-\text{O}-\text{NH}_2$ or $\textcircled{\text{P}}-\text{O}-\text{NH}_2$	R _i	Hydroxylamine	...
	R _{ii}	FMOC blocked amino acid	...
	R _{iii}	Sulfonylchloride	...

$\textcircled{\text{P}}$ = Solid support

Figure 3

Transformation

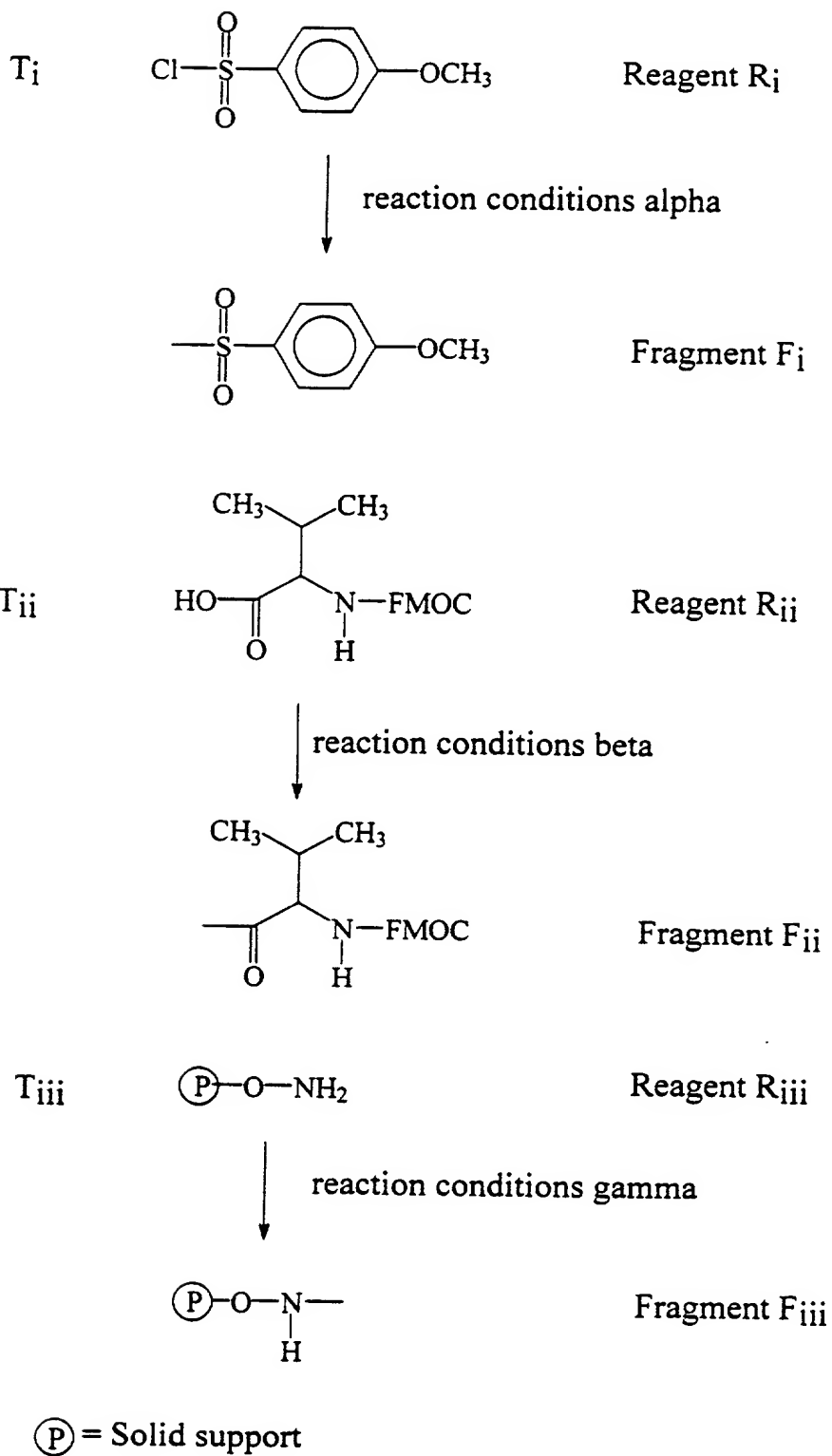


Figure 4

Common Fragment / Different Reagents and Transformations

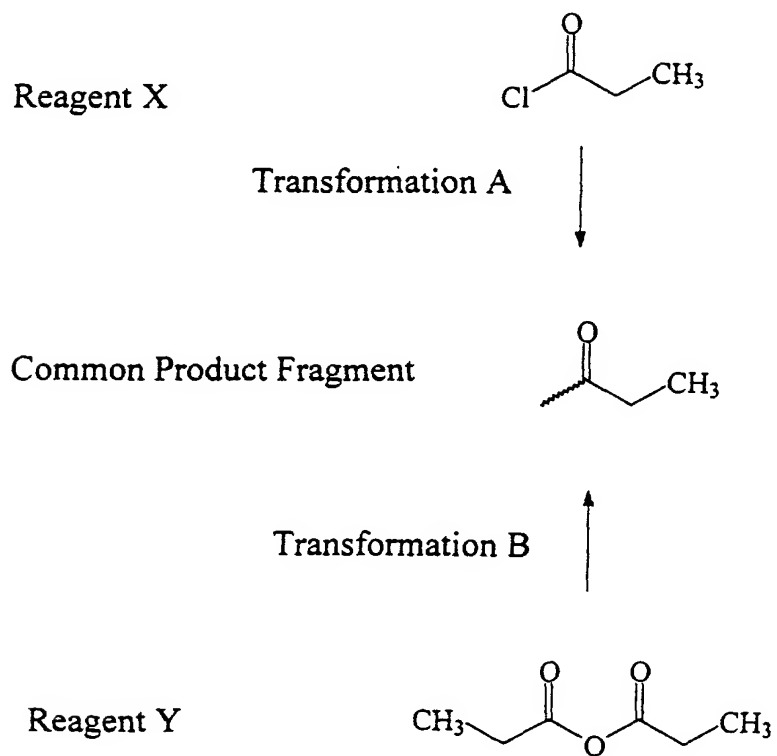


Figure 5

Common Fragment / Different Reagents and Transformations

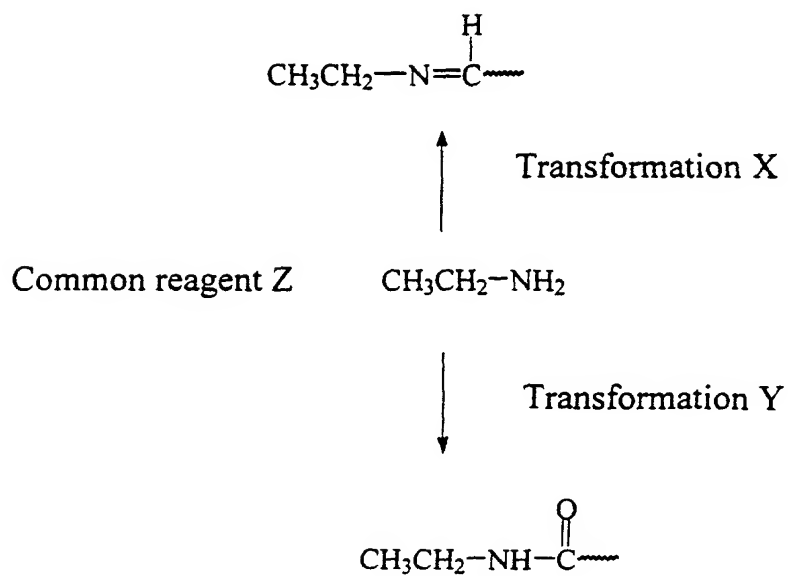


Figure 6a

Common Reagent

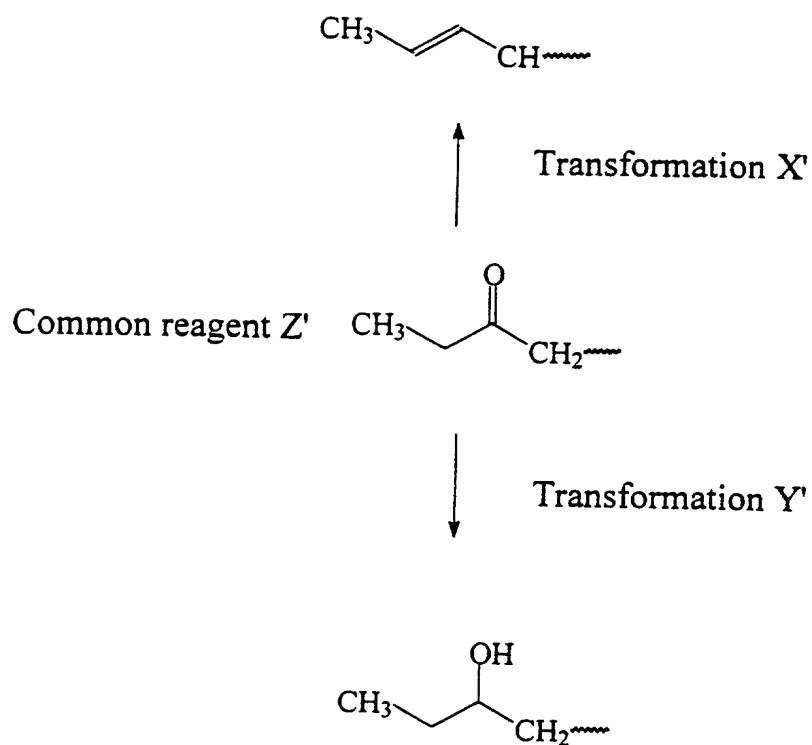


Figure 6b

Symbolic addition of fragments to yield compound



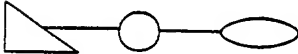
<u>Symbolic Structure</u>	<u>Symbolic Identifier</u>	<u>Molecular formula</u>
Fragment		
	F_i'	$C_uH_vN_w \dots$
	F_{ii}'	$C_uH_vN_w \dots$
$X - \bigcirc - Y$	F_{iii}'	$C_uH_vN_w \dots$
Compound		
	CI'	$C_uH_vN_w \dots$
		$ \begin{array}{r} \text{Molecular formula } F_i' \\ + \\ \text{Molecular formula } F_{ii}' \\ + \\ \text{Molecular formula } F_{iii}' \\ \hline = \text{Molecular formula } CI' \end{array} $

Figure 7

Symbolic Reagent Table


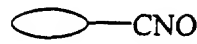


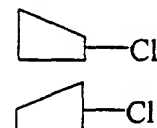
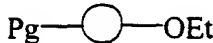

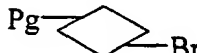
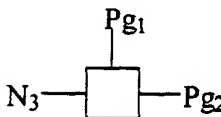
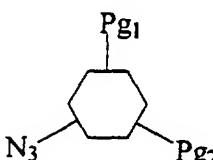
<u>Identifier</u>	<u>Name</u>	<u>Structure</u>	<u>Molecular formula</u>
R1	xxx		xxx
R2	...		...
R3	...		...
R4	...		...
R5	...		...
R6	...		...
R7	...		...
R8	...		...
R9	...		...
R10	...		...

Figure 8

Symbolic Fragment Table




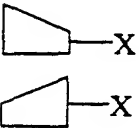

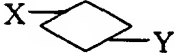
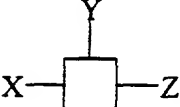
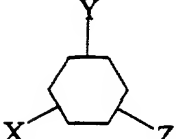
<u>Identifier</u>	<u>Symbolic Structure</u>	<u>Molecular formula</u>	<u>Molecular Weight</u>
F1		xxx	xxx
F2	
F3	
F4	
F5	
F6	
F7	
F8	

Figure 9

Symbolic Transformation Table

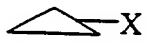
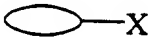


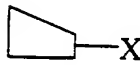
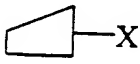


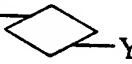
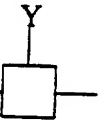
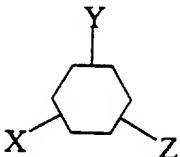
<u>Identifier</u>		<u>Symbolic Reactions</u>	<u>Reagent</u>
T1	F1	 ← R1	conditions α
T2	F2	 ← R2	conditions β
T3	F3	 ← R3	conditions α
T4	F3	 ← R4	conditions α
T5	F4	  ← R5	conditions α
T6	F5	X—  —Y ← R6	conditions ε
T7	F5	X—  —Y ← R7	conditions α
T8	F6	X—  —Y ← R8	conditions α
T9	F7	X—  —Z ← R9	conditions γ
T10	F8	X—  —Z ← R10	conditions γ

Figure 10

Single Compounds and Mixtures

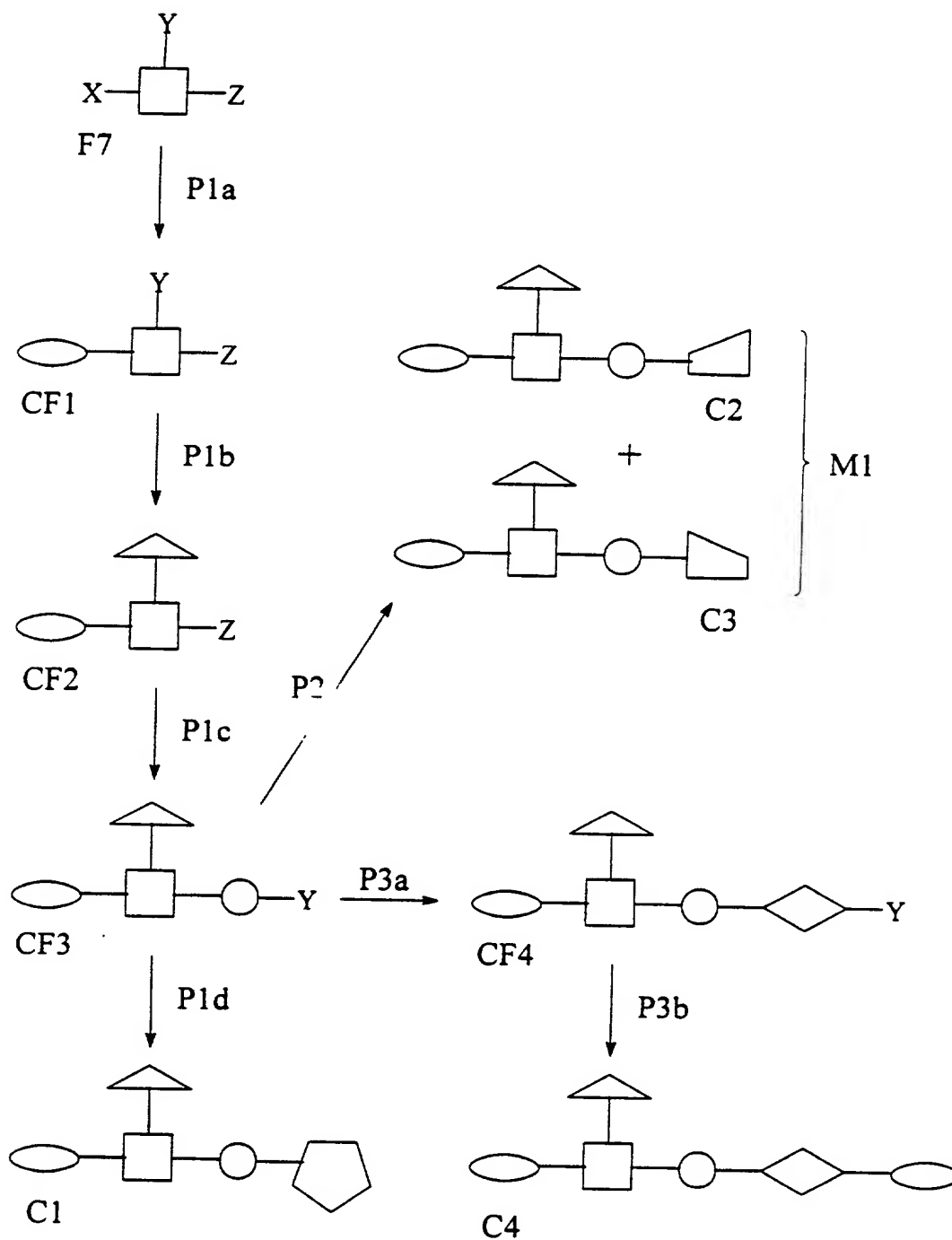


Figure 11

Mixture 2

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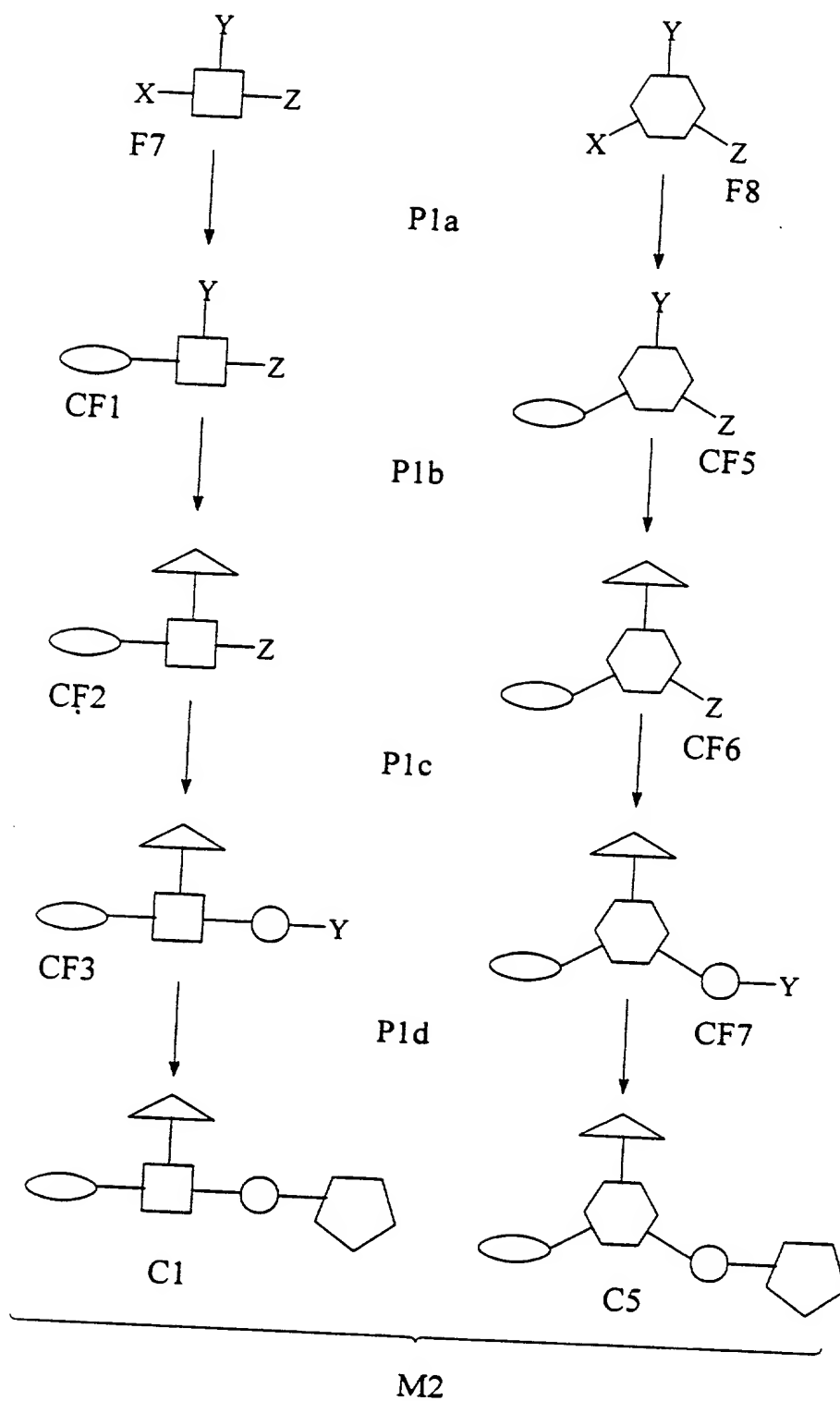


Figure 12

Mixture 3

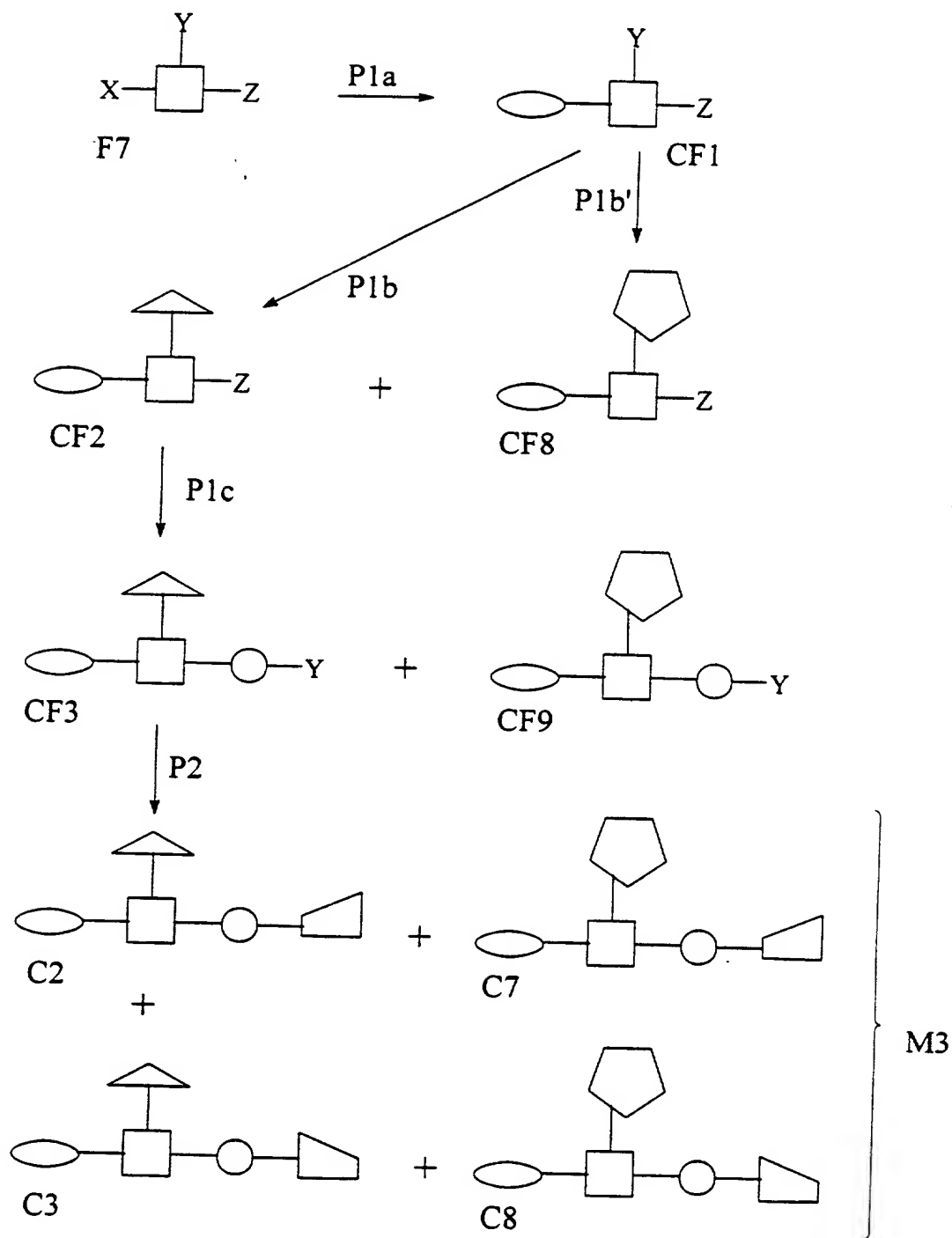
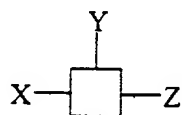


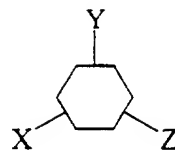
Figure 13

Mixture 4

2 Starting Fragments

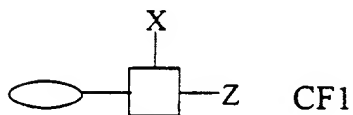


F7

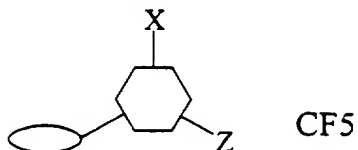


F8

2 Complex Fragments

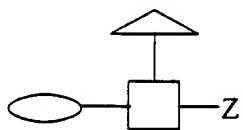


CF1

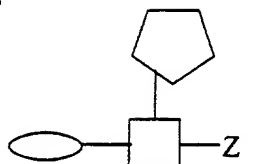


CF5

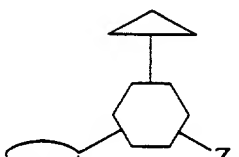
4 Complex Fragments



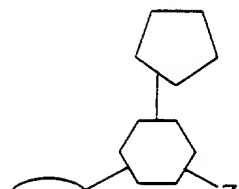
CF2



CF8

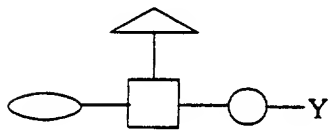


CF 6

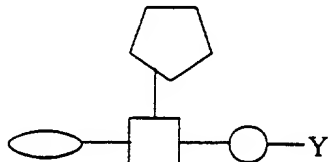


CF11

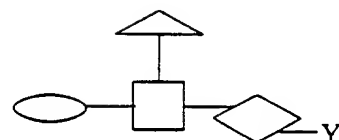
8 Complex Fragments



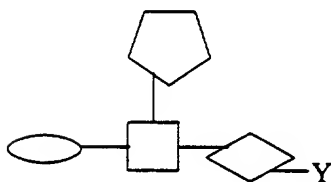
CF3



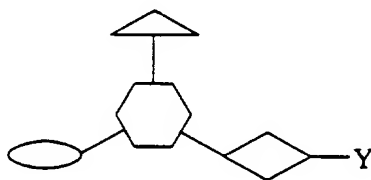
CF9



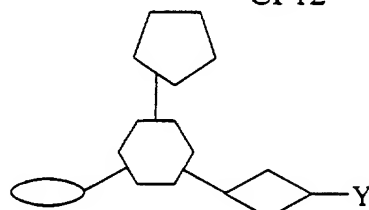
CF12



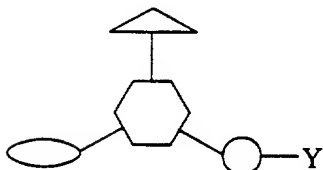
CF13



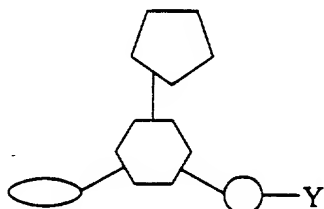
CF15



CF16



CF 7



CF14

Figure 14a

Mixture 4 (continued)

16 compounds

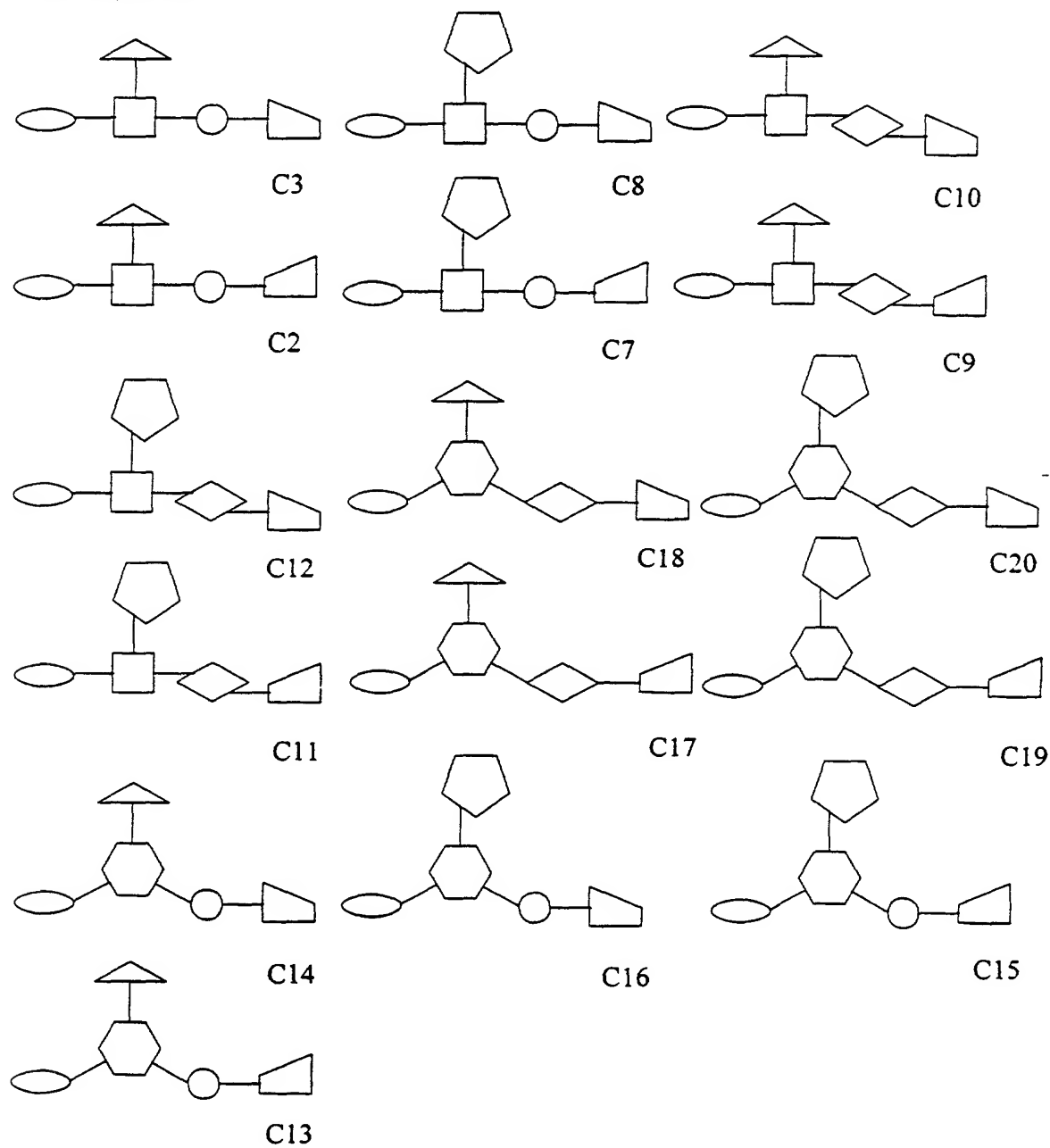


Figure 14b

Tracking Table for Compound C1

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(a) By Fragments:

n	n+1	n+2
F7	F2 F1 F5	F3

(b) By Transformations:

Synthesis Path 1

n	n+1	n+2
T9	T2 T1 T6	T3

Synthesis Path 2

n	n+1	n+2
T9	T2 T1 T7	T3

Synthesis Path 3

n	n+1	n+2
T9	T2 T1 T6	T4

Synthesis Path 4

n	n+1	n+2
T9	T2 T1 T7	T4

Figure 15

Tracking Table

Tracking M1

Step 1		
T9		
Step 2		
T9	T2	
Step 3		
T9	T2 T1	
Step 4		
T9	T2 T1 T7	
Step 5		
T9	T2 T1 T7	T5 ¹
C2		
Step 5		
T9	T2 T1 T7	T5 ²
C3		

Figure 16

Tracking Table

Tracking M2

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Step 1		
n	n+1	n+2
T9		

Step 1		
n	n+1	n+2
T10		

Step 2		
n	n+1	n+2
T9	T2	

Step 2		
n	n+1	n+2
T10	T2	

Step 3		
n	n+1	n+2
T9	T2 T1	

Step 3		
n	n+1	n+2
T10	T2 T1	

Step 4		
n	n+1	n+2
T9	T2 T1 T7	

Step 4		
n	n+1	n+2
T10	T2 T1 T7	

Step 5		
n	n+1	n+2
T9	T2 T1 T7	T4

Step 5		
n	n+1	n+2
T10	T2 T1 T7	T4

C1

C5

Figure 17

Tracking Table

Tracking M3

Step 1

T9		
----	--	--

Step 2

T9	T2	
----	----	--

Step 3

T9	T2 T1	
----	----------	--

Step 3

T9	T2 T3	
----	----------	--

Step 4

T9	T2 T1 T7	
----	----------------	--

Step 4

T9	T2 T3 T7	
----	----------------	--

Step 5

T9	T2 T1 T7	
----	----------------	--

T5¹

C2

Step 5

T9	T2 T1 T7	
----	----------------	--

T5²

C3

Step 5

T9	T2 T3 T7	
----	----------------	--

T5¹

C7

Step 5

T9	T2 T3 T7	
----	----------------	--

T5²

C8

Figure 18